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Thermo-Gas-Dynamic Model of Afterburning in Explosions

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A theoretical model of afterburning in explosions created by turbulent mixing of the detonation products from fuel-rich charges with air is described. It contains three key elements: (i) a thermodynamic-equilibrium description of the fluids (fuel, air, and products), (ii) a multi-component gas-dynamic treatment of the flow field, and (iii) a sub-grid model of molecular processes of mixing, combustion and equilibration.

Thermodynamic Model

The model recognizes four fluids: (i) air-*A*, (ii) fuel-*F* (expanded products gases from the detonation of fuel-rich condensed charges), (iii) frozen reactants-*R* (a stoichiometric mixture of *A* & *F*, in ratio: $\sigma_s = m_A/m_F$), and (iv) equilibrium combustion products—*P*. The thermodynamic states of these fluids were evaluated by the Cheetah code (Fried, 2003). Computed results are displayed in the form of a *Le Chatelier* diagram: locus of states of specific internal energy versus temperature presented in Fig. 1. The computed points were fit with least-squares polynomial functions:

$$\begin{aligned} u_A(T) &= -13.765 + 0.03502 * T + 7.5822 * 10^{-5} * T^2 & u_F(T) &= -1183.8 + 0.16214 * T + 6.3781 * 10^{-5} * T^2 \\ u_R(T) &= -292.34 + 0.065287 * T + 7.2955 * 10^{-5} * T^2 & u_P(T) &= -745.69 - 0.21279 * T + 18.262 * 10^{-5} * T^2 \end{aligned} \quad (1)$$

which are suitable for specifying the thermodynamic properties (equations of state) required by the Gasdynamic Model. The accuracies of these loci of states were confirmed by comparing the *F* and *P* curves with the heats of detonation and combustion (H_d and H_c), and species

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compositions as measured in bomb calorimeter experiments (Ornellas, 1984).

Gasdynamic Model

The model considers afterburning in the limit of large Reynolds, Peclet, and Damköhler number. At this limit, effects of molecular transport are negligible, and, the flow field is governed by the multi-component gas-dynamic conservation equations:

$$\text{Mass:} \quad \partial_t \rho_m + \nabla \cdot (\rho_m \mathbf{u}) = 0 \quad (2)$$

$$\text{Momentum:} \quad \partial_t \rho_m \mathbf{u} + \nabla \cdot (\rho_m \mathbf{u} \mathbf{u}) = -\nabla p_m \quad (3)$$

$$\text{Energy:} \quad \partial_t \rho_m (u_m + \mathbf{u} \cdot \mathbf{u} / 2) + \nabla \cdot \rho_m (u_m + \mathbf{u} \cdot \mathbf{u} / 2) \mathbf{u} = -\nabla \cdot (p_m \mathbf{u}) \quad (4)$$

$$\text{Components:} \quad \partial_t Y_k + \mathbf{u} \cdot \nabla Y_k = \alpha_k Y_s^* \quad \& \quad \sum_k Y_k = 1 \quad (k = F, A, P) \quad (5)$$

where ρ, u, p and \mathbf{u} denote the density, specific internal energy, pressure and velocity, respectively, Y_k is the mass fraction of component k ($Y_k \equiv \rho_k / \rho_m$) and subscript m denotes mixture. In the above, $\alpha_k = \{-1, -\sigma_s, (1 + \sigma_s)\}$ for $k = F, A, P$ represents the mass source/ sink strength, and σ_s denotes the stoichiometric air/fuel ratio ($\sigma_s = 3.2$ for TNT-air). Thus combustion acts simultaneously as a mass sink for F & A , and a mass source for P . For the case of afterburning of hot detonation products in air, kinetics are virtually instantaneous ($Da = \infty$), and Y_s^* becomes a delta function.

The above must be closed by *equations of state*: $p_k = f(\rho_k, u_k)$. Based on the quadratic relations $u_k(T_k) = a_k T_k^2 + b_k T_k + c_k$ of (1) and the perfect gas law, one has for a pure component k :

$$T_k = [-b_k + \sqrt{b_k^2 - 4a_k(c_k - u_k)}] / 2a_k \quad (6)$$

$$p_k = \rho_k R_k T_k \quad (7)$$

while for a mixture m one finds

$$T_m = [-b_m + \sqrt{b_m^2 - 4a_m(c_m - u_m)}] / 2a_m \quad (8)$$

$$p_m = \rho_m R_m T_m \quad (9)$$

where the mixture properties are determined from the thermodynamic mixing rules

$$a_m = \sum_k Y_k a_k \quad \& \quad b_m = \sum_k Y_k b_k \quad \& \quad c_m = \sum_k Y_k c_k \quad \& \quad R_m = \sum_k Y_k R_k \quad (10)$$

Combustion Model

This models the sub-grid molecular processes of mixing, combustion, and thermal equilibration that obey thermodynamic mixing rules based on mass and energy conservation depicted in Fig. 2. First, a stoichiometric mixture of reactants is formed (blue lines in Fig. 2):

$$\text{Mass:} \quad m_R = m_F + m_A \quad \text{where} \quad \begin{cases} m_A = \sigma_s m_F & \text{if } \sigma > \sigma_s \\ m_F = m_A / \sigma_s & \text{if } \sigma < \sigma_s \end{cases} \quad (11)$$

$$\text{Energy:} \quad u_R = (u_F + \sigma_s u_A) / (1 + \sigma_s) \quad (12)$$

Next comes combustion, which corresponds to material transformation from R to P (red lines):

$$\text{Mass:} \quad m_P = m_R \quad (13)$$

$$\text{Energy:} \quad u_P = u_R \quad (14)$$

And then, thermal equilibration between combustion products and diluent D (green/pink lines):

$$\text{Mass:} \quad m_m = m_P + m_D \quad (15)$$

$$\text{Energy:} \quad u_m = [m_P u_P + m_D u_D] / m_m \quad (16)$$

Application

The Model was used to simulate the explosion of a 0.875-kg cylindrical TNT charge in a 16.6- m^3 chamber. Evolution of the total energy in each fluid: $U_k = \int_{V_c} (u_k + \mathbf{u} \cdot \mathbf{u}/2) \rho_k dV$ is presented in Fig. 3; it shows that in this formulation, the total energy of the mixture (green line) is constant—a *system invariant*—throughout the combustion process. Computed pressure histories are in good agreement with measured pressure records. Further details of the flow field, including movies of the mixing and combustion, will be given in the presentation.

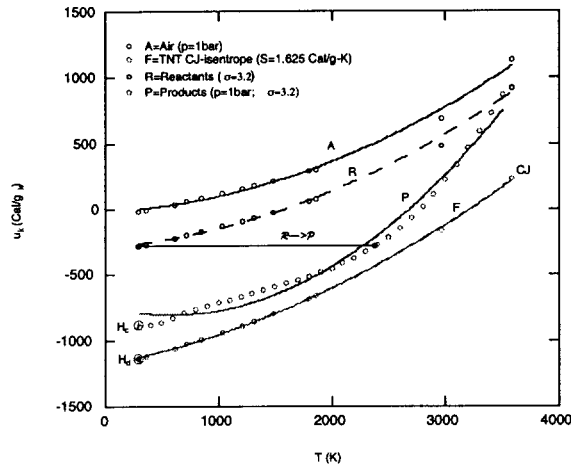


Figure 1. Le Chatelier diagram of afterburning of TNT products in air. In this Model, combustion in an enclosure corresponds to a *material transformation* (jump) from $R \rightarrow P$ at constant energy (black line).

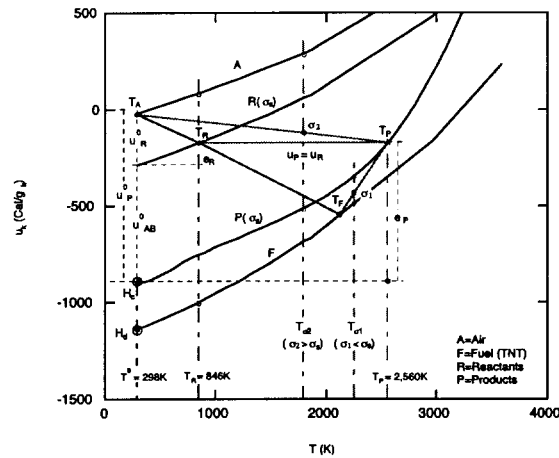


Figure 2. Combustion model: (i) reactants (blue), (ii) combustion (red), and equilibration (green/pink).

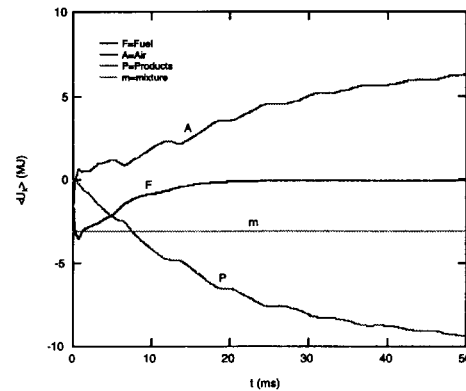


Figure 3. Total energy evolution in the fuel (black), air (blue), products (red) and mixture (green).